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Interpreting Geological Structure Using Kriging

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Abstract. We applied kriging (geostatistics) to interpret the structure of basement rock in Yucca Flat, NTS from borehole data. The estimation error for 118 data is 81 m comparable with those based on both gravity and borehole data. Using digitized topographic data, we tested the kriging results and found that the model validation process (Thomas option) on data gave a fair representation of the overall uncertainty of the kriged values.

Introduction

The understanding of subsurface structure is an essential part of exploration and the design of large scale underground structures. Generally most of the information is gathered from drill holes. These fragmentary data must be pieced together to obtain a complete picture for the whole area. Therefore some type of interpolation must be used to fill in between data. Since most geological information is spatially correlated, it is advantageous to use an interpolation technique that takes the spatial information into account. Kriging is one of the techniques having this property.

Principles of Kriging

Kriging is a statistical spatial estimation technique. It was named after D. G. Krige who originally applied the idea to the estimation of ore reserves in gold mines. The mathematical foundations of kriging were developed by G. Matheron (1971). Kriging consists of two parts: estimation of a variogram which describes the degree of correlation between any two observations as a function of the distance between them, and calculation of the kriging weights which indicate the relative influence of each data observation on the interpolations. A kriging estimate has two optimal statistical properties. First, it is unbiased. In other words, it reproduces the data value if there is no measurement error. Second, the kriging estimate is of minimum variance. Therefore, kriging may be considered as a weighted least-squares technique where the weights are calculated by minimizing the variance under the constraint of unbiasedness using the Lagrangian multiplier technique.

A variogram is a statistical model that describes the statistical property of a particular data set. By choosing a variogram for a data set, we tailor the kriging process to that specific data set. Kriging was designed under certain assumptions to produce estimates that minimize the difference between the true surface and the estimated surface for the whole region, not just at data points. This is because the optimum kriging weights depend only on the location of the data and the form of the variogram, not on the measured values themselves. In addition to the estimates kriging provides the standard deviation of the error, which is a measure of the uncertainty of the estimates.

In kriging, the observed value of the phenomenon is generally separated into two parts, i.e., a large scale trend called drift and a small scale fluctuation which the variogram tries to model. Figure 1 shows one of the variogram model where the variance is plotted as a function of distance between two data points. The parameters a and w are called range and sill. The range is the range of influence between two data points and the sill the maximum variability in the system. The nugget effect (c) is a parameter to describe a discontinuity at zero distance as in a gold mine where a gold nugget may be found at one place but not next to it. Not all variogram models have a sill. A linear variogram may extend indefinitely. However, short distance behavior of a variogram is much more important than behavior at longer distances.

Once we have identified the variogram and the drift and have calculated the kriging estimates and their associated uncertainties, we have to find a way to validate the model. The validation process is called Doubting Thomas. We remove one data point at a time and try to estimate the value and its associated uncertainty at the point using the rest of the data. We repeat the process for all data points and make statistical analyses of the results. Three criteria are used:

$$\sum_{i=1}^{N} [z^*(x_i)-z(x_i)] \approx 0$$

$$\sum_{i=1}^{N} [z^*(x_i)-z(x_i)]^2 \text{ is minimum,} \qquad (1)$$

and

$$\sum_{i=1}^{N} \left[\frac{z^*(x_i)-z(x_i)}{s^*(x_i)}\right]^2 \approx 1$$

where $z(x_i)$, $z^*(x_i)$, and $s^*(x_i)$ are the measured, the estimated values, and the estimated uncertainties at location x_i for N data points.

The first criterion says that the kriged average error should be close to zero. The second criterion says that the mean squared error should be at a minimum. The ratio of the kriged error and the uncertainty is called the standard error. If a model is good, the calculated uncertainty should reflect the calculated error, thus the ratio should be close to 1.

In addition to the overall consistency between the model and the data, we should also look for any local inconsistency. If the absolute value of the standard error for a particular data point is larger than 2.5, then we should double-check that point. It is quite possible that the data point is bad or that some local discontinuity, such as a fault, is in the vicinity.

Application to NTS Subsurface Geology

Lawrence Livermore National Laboratory has several working kriging codes. We applied kriging to various geological and physical parameters from drill hole data at Yucca Flat, Nevada Test Site (NTS) (Mao 1983). Yucca Flat is an intermontane basin measuring about 30 km N-S and about 12 km E-W. It is located about 100 km northwest of Las Vegas. We will concentrate on the study of the depths to the top of the surface of pre-Cenozoic basement rock (Pz) at Yucca Flat to demonstrate the methodology of kriging.

There are 118 data of Pz ranging from 40 to 1085 m deep at Yucca Flat within the study area (Figure 2). All the data are treated as exact during the calculation. Although there are many faults in the region, only the Yucca Fault is included in the estimation.

The depths to the top of Pz at Yucca Flat was interpreted by Healey (1977) based on both gravity and drill hole data. Brethauer and his colleagues (Brethauer et al., 1981) compared 38 observations of the depth to Pz in Yucca Flat with those calculated using surface gravity and borehole data. On average, the gravity method tends to overestimate the depth to Pz by 30 m, and the standard deviation of the estimates is 88 m. Brethauer et al., attributed the overestimation to sampling bias that results from the depth-of-drilling philosophy associated with the drilling of exploratory or emplacement drill holes. Use of the estimates for 17 exploratory holes only reduced the mean of the differences to +3.5 m with a standard deviation of 75.2 m.

Since gravity data do not give a unique solution, the final model often is influenced strongly by other geophysical and geological data. It is possible that the depth accuracy of ~80 m is primarily controlled by the borehole data alone with little influence from gravity data. We applied kriging to Pz from borehole data alone to demonstrate this point.

By using the automatic structure identification option (Reco), we obtained a linear drift model with a linear variogram. The mean difference for 118 data is -4.1 m with a standard deviation of 98 m. Alternatively we can assume a variogram model first. The standard deviation obtained by the Thomas option is then used to adjust the coefficients of that particular variogram model through trial and error. We do this for different variogram models and drift models. The one that gives the smallest standard deviation is chosen as "the model".

Following this procedure, we found that the smallest standard deviation for the 118 data points is 81 m from a power law variogram of the following form,

$$\gamma = 2.64\ h^{1.15} \qquad (2)$$

with the major anisotropic axis at N20°W and a ratio of 2.90, where γ is the variance and h is the distance. The ratio of anisotropy is basically a scaling factor for h when measured normal or parallel to the major axis. This model together with a constant drift and the location of the Yucca Fault was used to generate a 29 x 26 regular grid for the contour plots and the uncertainty map (Figure 3).

Table 1 summarizes the basic statistics of the estimated and measured depths to Pz at Yucca Flat from various approaches. The best kriging results from 118 borehole data give a mean of -0.7 m and a standard deviation of 81 m, comparable with that obtained by gravity method. Since kriging uses borehole data alone (except the location of Yucca Fault), it implies that the historical depth uncertainty of ~80 m is most likely a function of relief on the buried surface. Brethauer et al. (1981) also observed that there was no correlation between the difference of estimated and measured depth with the measured depth. This observation is contrary to the general belief that the uncertainty of a depth estimate from gravity data increases with depth. The scatter diagrams (Figure 4) from kriging also shows no depth dependence. All these lead to the conclusion that the uncertainty of depth estimates using gravity method is controlled mainly by the Pz tags. For an area where the borehole data are sparse, the gravity estimate might have the edge.

Kriging Test

In general, the only information we have are the values at the data points. Under these circumstances, the validation process of the Thomas option is the best we can do to check the consistency between the models (both drift and variogram models) and the data. We assume that the results of the Thomas option represent the average uncertainty for the entire data area, not just at the data points. The validity of this assumption can only be checked if we know the "truth". The kriging test was attempted to answer this question.

We selected an area where digitized topographic data are available and the relative relief is similar to the Pz surface at NTS. There are 200 x 200 digitized data points on a regular grid within a 12 km x 12 km area. This is our ground truth. From the 200 x 200 grid points we selected a 40 x 40 regular grid as our reference. Next, we randomly selected 5 data sets varying from 50 points to 400 points. We applied kriging to each data set to recreate the reference surface. The kriged 40 x 40 grid points are contoured and compared with the reference values. The RMS of the differences are also calculated. Figure 5 shows the contour map of the reference surface together with those kriged from 400, 200, 150, 100, and 50 data points. As expected, the detail in similarity decreases as the number of data points decreases. The important fact is that the vital features are reserved even for the case of only 50 data points.

Intuitively, we may assume that the standard deviation of the differences between the kriged 40 x 40 grid values and the reference values (the truth) must be a function of the number of data points and the variance of the true surface. Since generally we do not know the truth, we assume that the data variance represents the true variance. Kriging test results are summarized in Table 2 where the corresponding RMS error of the Thomas option results are also listed. In general, the standard deviations of the differences of 1600 points are in good agreement with the RMS error obtained from the Thomas option for various data sets except the case of N = 150 where the RMS error from the Thomas option is much better. In fact, it is better than that for N = 200 and is comparable to that for N = 400. The results of the Thomas option may be influenced by the distribution of the data point. In an extreme case, if all data points are distributed in pairs of identical value, the results of the

Thomas option will be deceivingly good. This is because by removing one point there is always another point nearby with an identical value to influence the estimate. We believe that the small RMS error for N = 150 is fortuitous. A semi logarithms plot between the number of data points and the standard deviation of the differences between the reference values and the kriged values normalized by the data variance shows a linear relationship (Figure 6) as

$$S.D. = \sigma\,(0.69 - 0.22 \log N) \qquad (3)$$

Two sets of values are plotted in Figure 6. The crosses are directly from the Reco option. Since the RMS error of the Thomas option for N = 150 is exceptionally low, we also used that particular generalized covariance model for other data sets (circles in Figure 6). The difference between the two sets of values are small.

For Pz depths in Yucca Flat, there are 118 data points. However, the Yucca Fault divides the area into two parts. There are 68 data points west of Yucca Fault and 50 data points east of Yucca Fault. The variance for the data is about 70000 m^2. The S.D. calculated from above equation is 76 m for the west side and 84 m for the east side with a weighted average of 80 m for the total area. This is in very good agreement with the RMS error of the Thomas option of 81 m.

Summary and Conclusion

We have demonstrated that kriging can be applied to interpret geological structure. However, there are several directions worth further research. First, the results of the Thomas option represent the average uncertainty for the whole area. For certain applications we want to optimize the estimate locally. In other words we want to validate the model with all the data but within a subarea. Second, dip/strike of a geological contact can provide additional information for the estimation of subsurface structure. The simplest way to implement these data is to construct a surface consistent with both the depth and the dip/strike data and redefine 3 points on the surface near the hole as our new data points (Delfiner et al. 1983). By forcing the estimated surface to go through these 3 points, it is more likely to conform to the true surface. Third, seismic and gravity data may be combined with borehole data to improve estimates (Delfiner et al. 1983). In general, these geophysical data can provide information about the large scale trend for the whole area and be tied down at each borehole location.

The results from the kriging test indicate that the Thomas option result is a fair representation of the overall uncertainty of the kriged values.

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Table 1.
Summary of Statistics of the Difference of Estimated and Measured Pz Depth in Yucca Flat

Method	No. of Observations	Mean (m)	S.D. (m)	Reference
Gravity (All Holes)	38	30.1	88	Brethauer et al., 1981
Gravity (Explor. Holes)	17	3.5	75	Brethauer et al., 1981
Next Hole (h 500 m)	56	-	85	This study
Next Hole (h 1800 m)	114	-	228	This study
Kriging (Reco)	118	-4.1	98	This study
Kriging (Best Model)	118	-0.7	81	This study

Table 2.
Kriging Test Results: Truth Minus Kriged Result (PLT40 - IRXXA)

No. of Data N	S.D. (m)	Data Variance σ^2 (m^2)	$\frac{S.D.}{\sigma}$	Log N	Thomas Option RMS (m)
50	107.6	103435	0.335	1.70	105.4
100	83.4	106553	0.252	2.00	76.8
150	77.2	119800	0.223	2.18	55.7
200	67.1	124116	0.190	2.30	65.2
400	51.4	130658	0.142	2.60	54.4

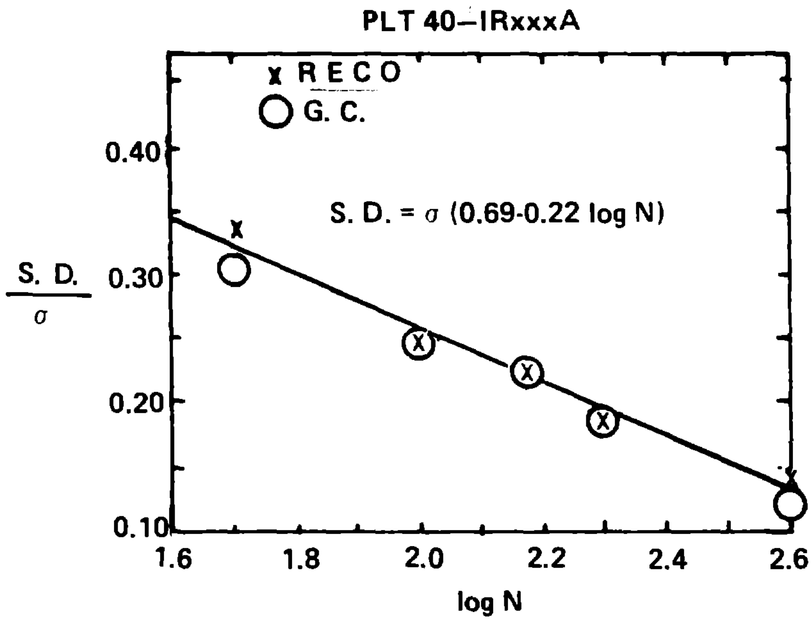

Figure 1. Spherical variogram model.

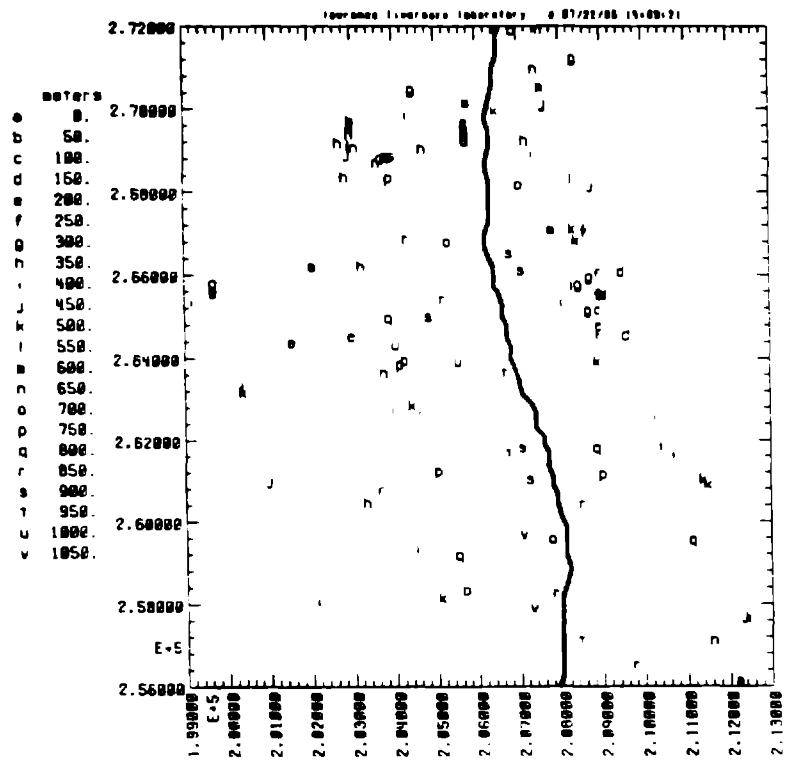

Figure 2. Location of Pz depth data.

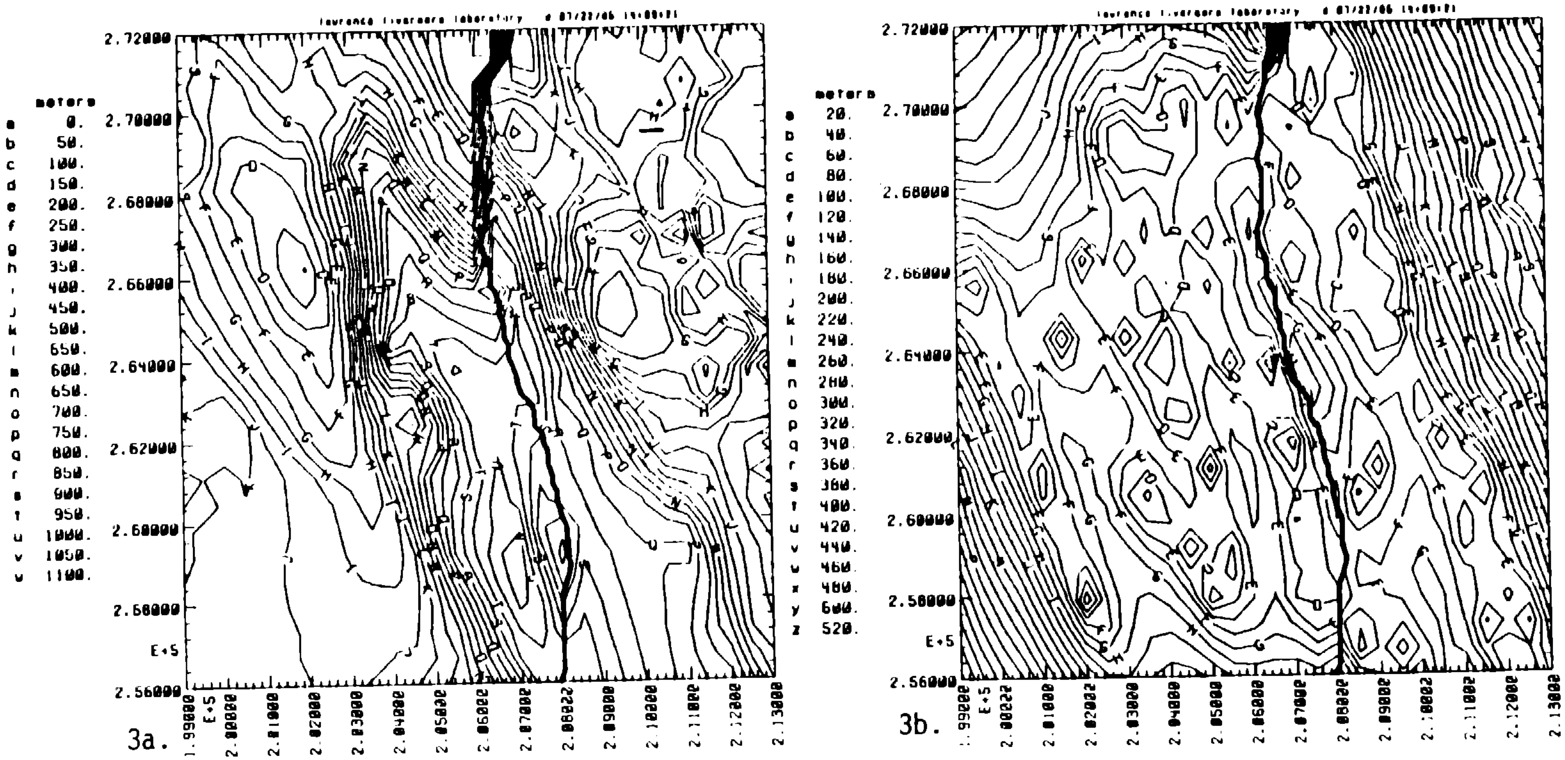

Figure 3. Kriged Pz depth (a) and uncertainty (b).

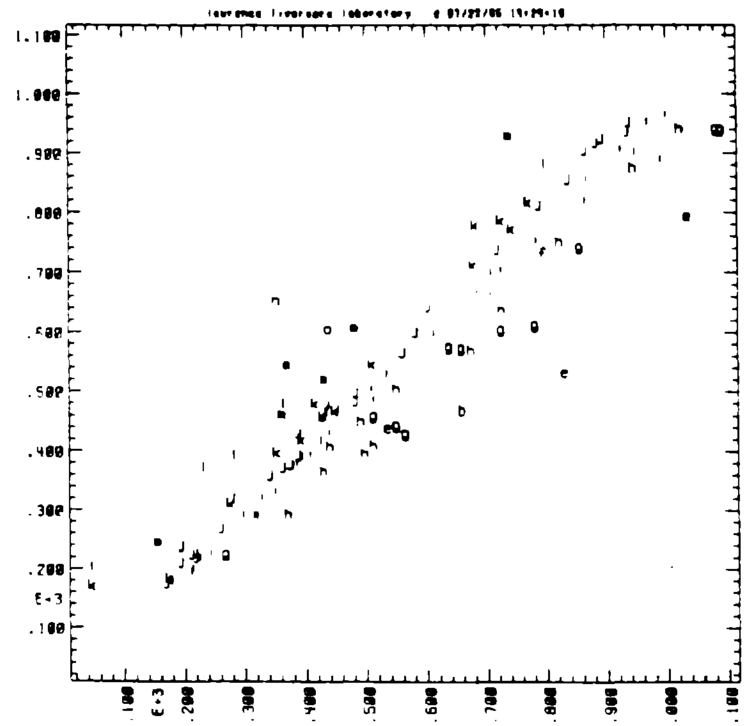

Figure 4. The estimated Pz depth vs measured.

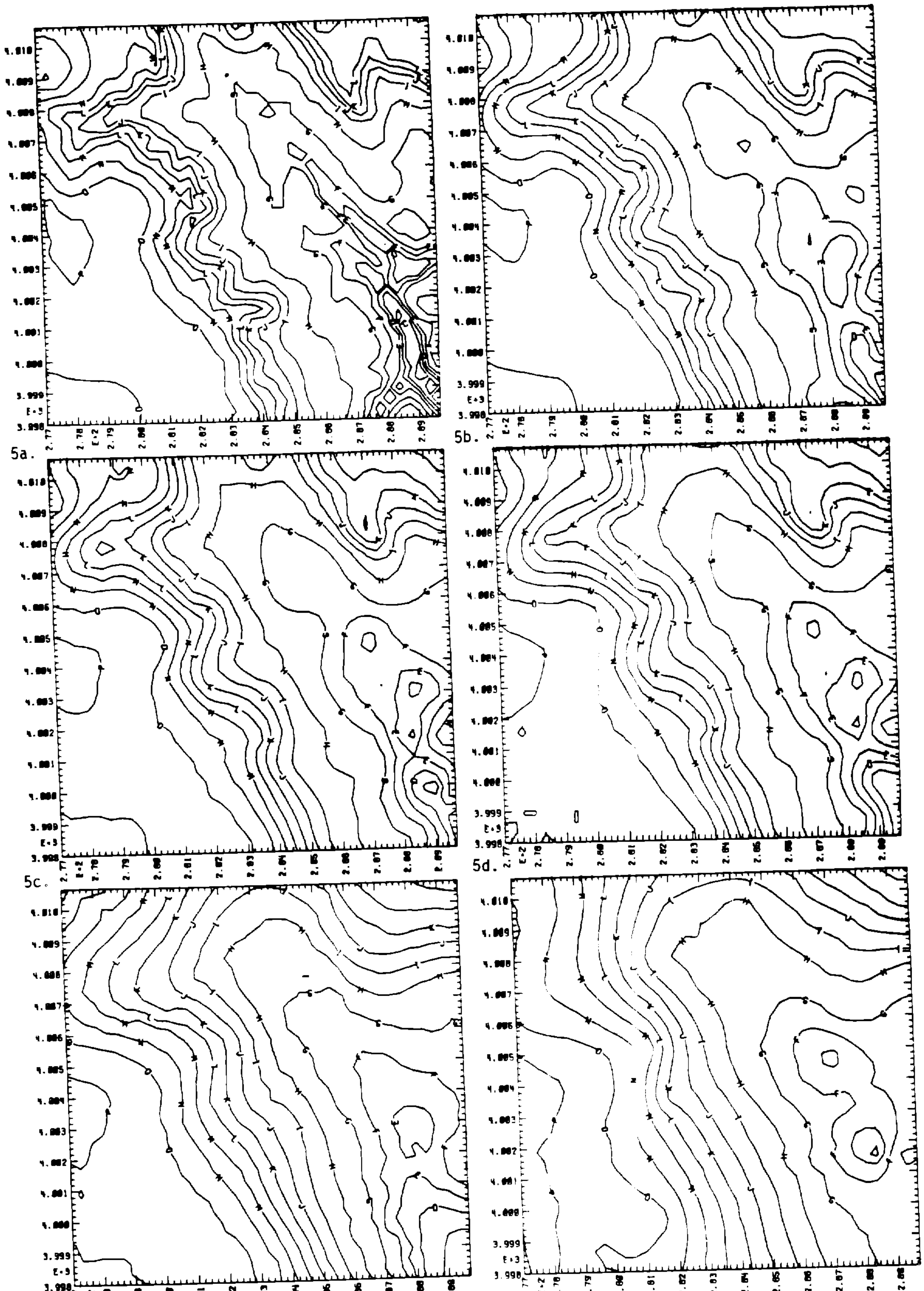

Figure 5. Comparison of results of kriging test:
a. "truth", b. 400, c. 200, d. 150, e. 100, and f. 50 data.

$$\gamma(h) = 0 \qquad h = 0$$
$$\gamma(h) = \omega[1.5h/a\text{-}0.5(h/a)^3] + c \qquad 0 < h = < a$$
$$\gamma(h) = \omega + c \qquad h = > a$$

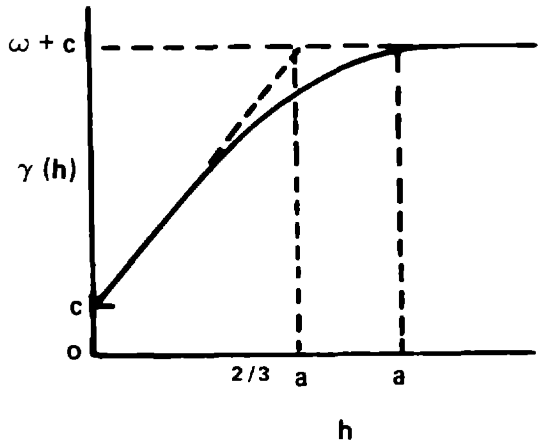

Figure 6. Kriging test results = $\frac{S.D.}{\sigma}$ vs log N.